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SHOCK SYNTHESIS OF NEW ALUMINUM OXIDE MODIFICATIONS USING AN OCTOGEN – ALUMINUM HYDRIDE MIXTURE

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The results of an x-ray diffraction study of two new modifications of aluminum oxide with tetragonal and hexagonal cells, synthesized by means of in an explosion of an octogen – aluminum hydride mixture (90/10 wt.%), are presented. The parameters of the tetragonal and hexagonal cells are, respectively, $a = 7.932(6)$ Å, $c = 9.142(5)$ Å, $c/a = 1.153$, $V = 575$ Å^3 and $a = 9.140(3)$ Å, $c = 3.980(4)$ Å, $c/a = 0.453$, $V = 288$ A^3. Matrices for transforming one set of cell parameters into the other are presented.

Key words: aluminum oxide, explosive synthesis, unit cell parameters, transformation matrix for lattice parameters.

A new modification of aluminum oxide λ-Al_2O_3 has been discovered by means of x-ray diffraction analysis of the condensed products of an explosion of a mixture of gibbsite with hexagen [1]. The character of the arrangement of the lines and the ratio of the intensities in the x-ray diffraction pattern of λ-Al_2O_3 made it possible to use the homology method to index the lines. A hexagonal lattice corresponding to hexagonal close packing was taken as the basis for the initial lattice. The type of distortion corresponded to the *C*-base-centered orthorhombic lattice. The transformation to an orthorhombic lattice is described by a matrix of the following form:

$$\begin{vmatrix} 1 & -1 & 0 \\ 1 & 1 & 0 \\ 0 & 0 & 1 \end{vmatrix}.$$

All lines of the x-ray diffraction pattern of λ-Al_2O_3 were indexed in the *C*-base-centered rhombic cell with $a = 8.501(6)$ Å, $b = 5.185(3)$ Å, $c = 6.146(4)$ Å, $V = 270.9(3)$ Å^3. It is possible to transform from this cell to a *P*-monoclinic cell with half the volume: $a = 4.979(6)$ A, $b = 6.146(4)$ Å, $c = 4.979(4)$ Å, $\beta = 117.24°$, $V = 135.5(3)$ Å^3.

The parameters a and c of λ-Al_2O_3 are somewhat larger than the parameter a of the α-Al_2O_3 cell ($a = 4.758$ Å, $c = 12.991$ Å), and the parameter b is approximately 2 times smaller than the parameter c in corundum.

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The possible combinations of the indices H_M, K_M, and L_M that correspond to the indices of a monoclinic lattice can be found by means of the transformation matrix:

$$\begin{vmatrix} H_M \\ K_M \\ L_M \end{vmatrix} = \begin{vmatrix} 0.5 & 0.5 & 0 \\ 0 & 0 & -1 \\ -0.5 & 0.5 & 0 \end{vmatrix} \begin{vmatrix} H_P \\ K_P \\ L_P \end{vmatrix}.$$

A new modification of aluminum oxide $Al_{8/3}O_4$ with a structure that derives from spinel was synthesized in previous work [2, 3] under a shock from the explosion of an octogen – aluminum mixture (90/10 wt.%). The x-ray diffraction pattern of this oxide was indexed in a primitive hexagonal cell with $a = 7.941(2)$ Å, $c = 4.575(1)$ Å, $c/a = 0.576$, $V = 288$ Å^3. The tetragonal cell is associated with a primitive hexagonal unit cell with twice the volume: $a = 9.151(1)$ Å, $c = 7.945(2)$ Å, $c/a = 0.868$, $V = 576$ Å^3.

All lines of the x-ray diffraction pattern of synthesized aluminum oxide can likewise be indexed in the parameters of a hexagonal cell.

The matrix for transforming from the tetragonal to hexagonal vectors has the form:

$$\begin{vmatrix} 0 & 0 & -2 \\ -1 & 0 & 1 \\ 0 & 1 & 0 \end{vmatrix}.$$

Next, we substituted aluminum hydride AlH_3 for aluminum in the explosive mixture. Additional x-ray diffraction data were obtained by a shock from an octogen – aluminum

TABLE 1.

I	d_e, Å	*hkl* tetragonal lattice	*hkl* hexagonal lattice
32	2,81049	220	201
58	2,39128	222	211
46	2,28590	004	220
87	1,98006	204	400
5	1,93825	313	–
9	1,82513	–	112
22	1,52387	006	330
100	1,40009	216	421
7	1,03162	446	612

hydride mixture (90/10 wt.%) with the technique described in [2, 3]. The x-ray diffraction investigations were performed with monochromatized Cu$K_{\alpha 1}$ radiation in a "Huber Imaging Plate Guiner Camera."

The indexing results are presented in Table 1. It follows from the data in this table that the diffraction lines correspond to a two-phase sample with tetragonal and hexagonal cells.

The parameters of the tetragonal cell are: $a = 7.932(6)$ Å, $b = 9.142(5)$ Å, $c/a = 1.153$, $V = 575$ Å^3; the parameters of the hexagonal cell are $a = 9.140(3)$ Å, $b = 3.980(4)$ Å, $c/a = 0.435$, $V = 288$ Å^3.

The parameters c and a are practically equal in the tetragonal and hexagonal cells, and the parameter c of the hexagonal cell is half the parameter a of the tetragonal cell.

Therefore, a matrix of the following form corresponds to a transformation of the parameters from the tetragonal to hexagonal cells:

$$\begin{vmatrix} 0 & 0 & -1 \\ -1 & 0 & 0.5 \\ 0 & 0.5 & 0 \end{vmatrix}.$$

The transformation matrix from the hexagonal to the tetragonal cell is

$$\begin{vmatrix} -0.5 & 0.5 & 0 \\ 0 & 0 & -2 \\ -1 & -1 & 0 \end{vmatrix}.$$

In summary, using the shock from the explosion of an octogen – aluminum hydride mixture we have accomplished the first synthesis of two previously unknown modifications of aluminum oxide with a structure which is derived from spinel.

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